

# STUDY OF THE THERMAL AND MECHANICAL PROPERTIES OF $\text{La}_2\text{Zr}_2\text{O}_7$ USING FIRST PRINCIPLE METHOD

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As an advanced thermal barrier coating, Lanthanum zirconia ( $\text{La}_2\text{Zr}_2\text{O}_7$ ) has been studied in this paper using first principle calculations.  $\text{La}_2\text{Zr}_2\text{O}_7$  crystal bulk was used in this calculation. The lattice parameter, mechanical and thermal properties of  $\text{La}_2\text{Zr}_2\text{O}_7$  were investigated by means of density functional theory (DFT). Hydrostatic pressure-dependent elasticity constant, bulk modulus were calculated. The thermal conductivity was calculated based on Fick's law using a 20 layers supercell.  $\text{La}_2\text{Zr}_2\text{O}_7$  coating samples were sprayed by APS equipment, the coating samples were identified by XRD and observed by optical microscope. The thermal effect of Ce doping of the  $\text{La}_2\text{Zr}_2\text{O}_7$  were studied by ab initio calculations. The calculated properties have considerable good agreement with others experimental and calculation results.